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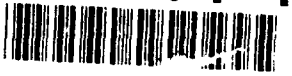

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13. ABSTRACT (Maximum 200 words)

We have continued our work on impact ionization including collisional broadening and the intracollisional field effect.

We have started to investigate the possibility of Monte Carlo simulations that use the pseudopotential form-factors as sole input to compute both band structure and phonon scattering rate and we have obtained preliminary results.

With regard to quantum transport, we have continued our work on phonon scattering in mesoscopic systems and we have obtained first numerical results on the electron-electron interaction in simple nanostructures.

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Impact ionization: beyond the Golden Rule

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Abstract. The influence of collision broadening due to phonons and the intra-collisional field effect on the inverse Auger process have been examined. Results are presented for silicon and show for the first time the wave-vector dependence of the ionization rate including collision broadening.

1. Introduction

Impact ionization (the exact inverse of the Auger process) in semiconductors has been studied extensively since the first theoretical investigations of hot carrier transport. An accurate description of the ionization process in solids requires a full band structure treatment along with associated constitutive complexities; inclusion of band structure effects requires detailed numerical calculations to establish the magnitude of the matrix elements for the process. Initial efforts to understand impact ionization did not consider detailed band structure effects, but developed simple phenomenological models. Prominent among initial studies of impact ionization was the Keldysh model [1], originally developed for direct gap, parabolic band materials; this model has been used extensively in applications.

Unfortunately, the Keldysh formula is not applicable for most real materials due to the complexities introduced by band structure effects; specifically, the formula does not adequately describe indirect gap materials such as silicon. Kane [2] has performed a more exact, Fermi Golden Rule calculation of the ionization process including a realistic band structure. However, the Fermi Golden Rule does not adequately describe the impact ionization process for two reasons; first, because the phonon scattering rate is typically very large for the high energy electrons which undergo impact ionization, the lifetime of the electron states is short, thereby broadening the ionization transition; secondly, electric fields are typically very large so that the ionizing electron can be accelerated considerably during the period of collision, thereby affecting the dynamics of the collision process.

In this paper a theory of impact ionization in semiconductors is presented which extends the initial work of Kane by including the influence of high electric fields and high scattering rates on the electron–electron collision process, and utilizes a more advanced treatment of band structure and dielectric response screening than was available to Kane in his original work [3]. Hence, the use of Monte Carlo methods combined with density matrix formalism results in a major extension of Kane's theory beyond the Golden Rule. In particular, this investigation shows that the already soft threshold of the ionization rate as indicated in Kane's theory is considerably broadened by electron–phonon collisions and the intra-collisional field effect, so that a well defined threshold does not exist. Furthermore, results show, for the first time, the wave vector anisotropy of the ionization rate in silicon; the importance of wave vector dependent thresholds is also discussed.

2. Quasi-particle Boltzmann equation for impact ionizing electrons

Many authors have attacked the problem of finding quantum transport equations which improve upon the Boltzmann equation in the high field limit [4]. In this section, we briefly outline a theory which includes the effects of the electric field and phonon scattering on impact ionization. A more detailed description is given in [3]. In order to incorporate the electric field, we choose a gauge based on the vector potential, namely (see for instance [5, 6]),

$$\boldsymbol{A}(t) = -c \int_0^t \boldsymbol{F}(t')\,\mathrm{d}t' \tag{1}$$

where $\boldsymbol{F}$ is the electric field and c is the speed of light. We can label our states with the usual Bloch band indices and accelerated Bloch wave-vectors $\boldsymbol{K}$ such that

$$\boldsymbol{K}(\boldsymbol{k}, t) = \boldsymbol{k} + \boldsymbol{E}_{\mathrm{F}} t \qquad \boldsymbol{E}_{\mathrm{F}} \equiv (e/\hbar)\boldsymbol{F} \tag{2}$$

where $\boldsymbol{k}$ is the usual Bloch wave-vector. This transformation allows an exact inclusion of the electric field. The Hamiltonian is written as

$$H_{\mathrm{tot}} = H_0 + H_{\mathrm{B}} + H_{\mathrm{AB}} + V \tag{3}$$

where H_0 contains the crystal potential and the electronic kinetic energy, H_{B} is the phonon bath Hamiltonian, H_{AB} is the system–bath interaction, and V is the

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electron–electron interaction corresponding to impact ionization.

Then, we look for an equation of motion for the diagonal of the electron density matrix which corresponds to the semi-classical distribution function. This is accomplished by applying the following projection operators (see for instance [7])

$$P = \frac{e^{-\beta H_B} tr_B}{tr_B e^{-\beta H_B}} \otimes \delta_{K',K} \qquad Q = 1 - P \tag{4}$$

to the equation of motion for the density matrix,

$$i\hbar \frac{\partial \rho}{\partial t} = [H_{tot}(t), \rho] \tag{5}$$

and back-transforming the result from the accelerated state basis to the stationary Bloch basis.

The resulting equation gives an expression for the impact ionization scattering rate $R(12 \to 34, t)$ from an initial state $|n_1k_1; n_2k_2\rangle$ to a final state $|n_3k_3; n_4k_4\rangle$, which includes virtual phonon processes and acceleration in the electric field. Note: for large t, $R(12 \to 34, t) \to R(12 \to 34)$. This exression replaces the energy conserving delta function of the Fermi Golden Rule:

$$R(12 \to 34, t) = \frac{2\mathrm{Re}}{\hbar^2} |V_{12;34}|^2 \int_0^t dt' \, S(12, 34; t, t') \tag{6}$$

$$\begin{aligned} S(12, 34; t, t') = \exp \frac{1}{\hbar} \Bigg[& i \int_{t'}^{t} dt'' \Bigg(\sum_{i=1}^{2} E_{n_i}(k_i - E_F(t - t'')) \\ & - \sum_{i=3}^{4} E_{n_i}(k_i - E_F(t - t'')) \Bigg) \\ & + i \Bigg(\sum_{i=1}^{2} \Delta(n_i, k_i) - \sum_{i=3}^{4} \Delta(n_i, k_i) \Bigg)(t - t') \\ & - \sum_{i=1}^{4} \Gamma(n_i, k_i)|t - t'| \Bigg]. \end{aligned} \tag{7}$$

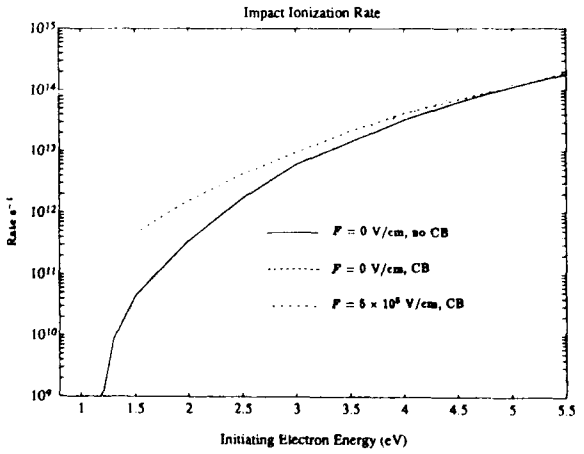

Figure 1. Impact ionization rates $R_{ave}(E)$ for Si averaged over initial electron energy measured from the bottom of the conduction band. Solid curve, zero field, no collision broadening; dotted curve, collision broadening (CB); chain curve, $F = 5 \times 10^6\,\mathrm{V\,cm^{-1}}$ and collision broadening.

Here $\Gamma(n_i, k_i)$ and $\Delta(n_i, k_i)$ are the imaginary and real parts of the electron self-energy (due to virtual phonons), and $|V_{12;34}|$ is the matrix element for the electron–electron interaction. The total scattering rate for an initial electron $R(n_1k_1)$ is given by

$$R(n_1k_1) = \sum_{34} R(12 \to 34) \tag{8}$$

and the rate averaged over initial electron energy, $R_{ave}(E)$, is

$$R_{ave}(E) = \frac{\Sigma_{n_1} \int_{BZ} d^3k_1 \, R(n_1k_1) \delta(E_{n_1}(k_1) - E)}{\Sigma_{n_1} \int_{BZ} d^3k_1 \, \delta(E_{n_1}(k_1) - E)}. \tag{9}$$

The expressions above are used to calculate the impact ionization rate for silicon under different field conditions.

3. Quantum effects and ionization thresholds

First, we examine the threshold dependence of $R_{ave}(E)$ for silicon. Figure 1 shows $R_{ave}(E)$ calculated using the Fermi Golden Rule, and deviations from the Fermi Golden Rule which occur because of the inclusion of either collision broadening alone, or from collision broadening and the intra-collisional field effect operative simultaneously; thus, deviations from the Fermi Golden Rule results are due to the inclusion of specific time dependent processes of finite time duration. The Golden Rule result shows a rapid, threshold-like increase in the scattering rate just below 1.5 eV; hence, $E_{th} \approx 1.5\,\mathrm{eV}$. However, when collision broadening is included, the 'threshold' decreases, allowing impact ionization to occur well below the silicon band gap. This clearly shows the influence of energy broadening due to the phonons. The ionization rate remains finite for energies down to 0.8 eV. Lower values of initial energy could not be computed because of numerical difficulties. For higher electron energies, the effect of collision broadening is relatively small; collision broadening has its greatest influence near thresholds where the rate increases rapidly with energy.

In the presence of high fields ($F = 10^5\,\mathrm{V\,cm^{-1}}$), the lower end of the ionization curve is broadened even more dramatically. Depending on the orientation of the electric field with respect to band structure, an impact ionizing electron can either gain or lose energy from the field during the period of a collision. The result is that low energy electrons, unable to impact ionize in the zero-field limit, can gain enough energy from the field during the time of the collision to ionize; this process can be viewed as an effective two-particle Franz–Keldysh effect. The effect is again most dramatic for electrons near the Golden Rule threshold.

4. Wave-vector dependent thresholds

Anderson and Crowell [8] were the first to consider the influence of crystallographic direction on threshold energy; an electron with a given initial wave-vector, $\boldsymbol{k}_i$,

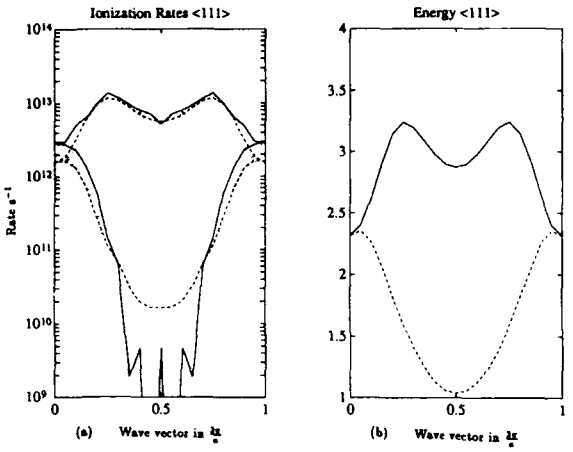

Figure 2. (a) Ionization rate in the ⟨111⟩ direction. Upper set of curves: second conduction band. Lower set: first conduction band. Solid lines, collision broadening $R(\boldsymbol{k})$; dotted, no collision broadening $R(\boldsymbol{k})$; chain, $R_{ave}(E(\boldsymbol{k}))$. (b) Energy in ⟨111⟩ direction; solid, second conduction band; dashed, first conduction band.

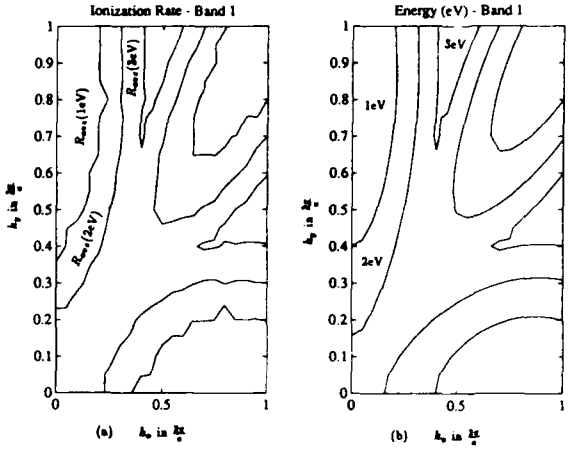

Figure 3. (a) Equal ionization rate curves in the $k_z = 0$ plane, first conduction band. (b) Equal energy curves in the $k_z = 0$ plane, first conduction band. The energy curves are in increments of 1.0 eV. The ionization rate contours correspond to the average rate for the equal energy surfaces $R_{ave}(1\,eV)$, $R_{ave}(2\,eV)$, etc.

can impact ionize only if its initial energy exceeds a minimum energy, $E_{th}(\hat{k}_i)$, where $\hat{k}_i$ is the unit vector in the k_i direction. Computations of $E_{th}(\hat{k}_i)$ in references [8] and [9] indicated a highly anisotropic threshold for Si of about 3 eV in the ⟨111⟩ direction while in the ⟨110⟩ and ⟨100⟩ directions thresholds of 2.1 eV and 1.1 eV were found. This means that rates with explicit $\boldsymbol{k}$ dependence, $R(\boldsymbol{k})$, could deviate significantly from $R_{ave}(E(\boldsymbol{k}))$. However, the above referenced calculations have assumed that the wave-vectors of the particles involved in threshold processes are all parallel to the initial particle wave-vector. This assumption is too restrictive, and overestimates the wave-vector anisotropy significantly.

In this paper, we have calculated $R(\boldsymbol{k})$ on a $0.05 \times 2\pi/a$ mesh in silicon, with and without collision broadening; the results of this calculation are shown in figures 2 and 3. Figure 2(a) shows $R(\boldsymbol{k})$ for the two lowest bands in silicon in the ⟨111⟩ direction. Even using the Fermi Golden Rule rates, there is a non-zero ionization rate for states with energy less than 1.5 eV. For the collision broadened case, the effective threshold is less than 1.2 eV. Figure 3(a) shows contours of equal ionization rate corresponding to the average ionization rate for the equal energy contours in figure 3(b). Here $k_z = 0$, and the states are in the first conduction band. The wave-vector anisotropy is small for most states in the $k_z = 0$ plane. This is verified in figure 3; here the average ionization rate contours follow the energy contours for almost all energies. We have found deviations of less than 25% from the $R_{ave}(E)$ even for states with $E < 2.0$ eV. However, the anisotropy becomes large below 1.5 eV, and may be play an important role for low fields.

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